OSCARS
Open Science Clusters' Action for Research & Society

Funded Project

Fail2Fair: Recovering Discarded Macromolecular Crystallographic Data

Implemented by

ibmb | CSIC | PSI | Universität Konstanz

Funded by the European Union

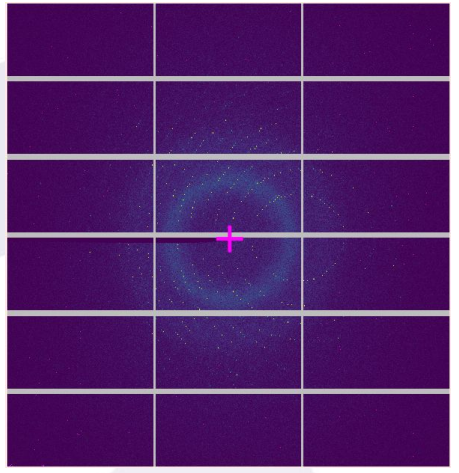
CHALLENGE ADDRESSED

- Macromolecular crystallography (MX) provides vital data for structure biology with applications in health and biotechnology
- Failed MX experiments are rarely archived
- Missing failed datasets limit method development and AI training
- Exponential increase in data rates for MX
- Archiving all X-ray images prohibitively expensive

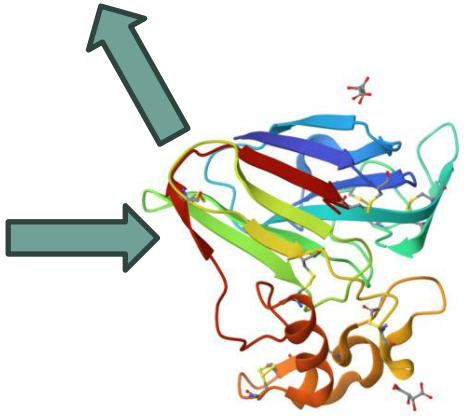
RCSB PDB PROTEIN DATA BANK

250,079 Structures from the PDB archive

1,068,577 Computed Structure Models (CSM)



X-ray diffraction images

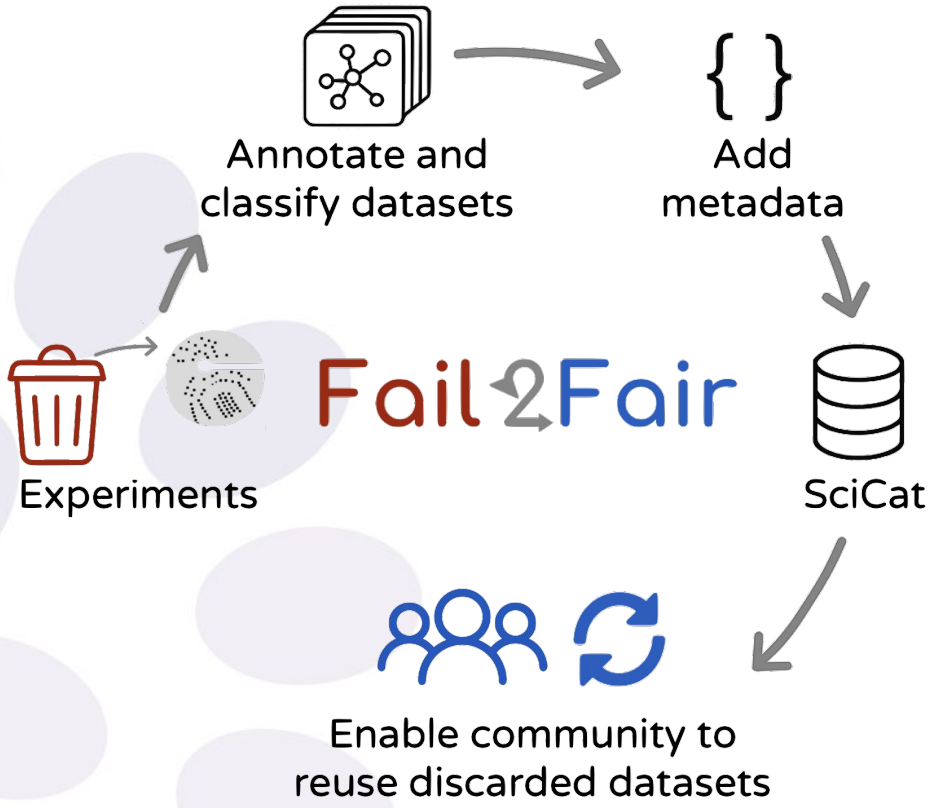


Protein structure

Synchrotron facility

SOLUTION

- Extend metadata models and automate dataset classification
- Compression to allow sustainable archiving and reuse of all datasets
- Engage community feedback and involvement with two workshops



RESULTS

- We will improve FAIR data availability at synchrotron facilities
- We will provide software to annotate datasets for common pathologies
- We will provide a proof of principle for scientific applications using these data

TEAM

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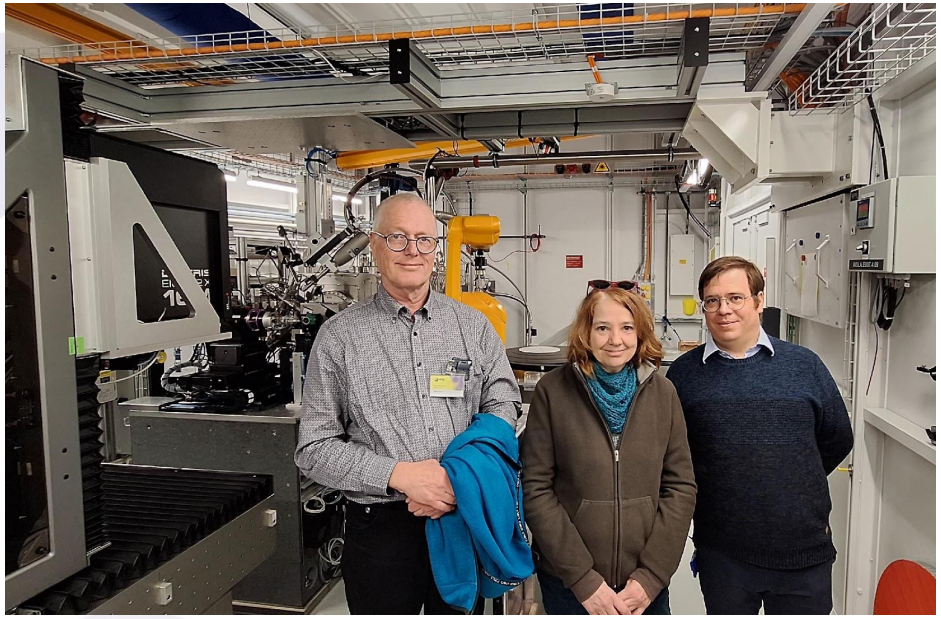
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